Fantastic plastic

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European Spallation Source

INSIDE MATERIALS

SEEING WITH NEUTRON EYES

How Europe's most advanced neutron facility will help in the understanding and development of new materials and their applications

02 THE EUROPEAN SPALLATION SOURCE

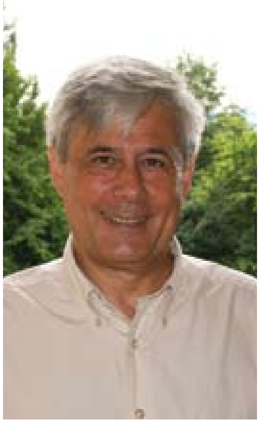
European Spallation Source

Europe's newest, most advanced neutron facility, the European Spallation Source (ESS), is to be built in Sweden. It will provide intense beams of neutrons and high-quality instruments for experiments across a wide range of research disciplines in both fundamental science and technologically important fields – from electronics and materials science to biomedicine and environmental science.

The ESS will benefit from being located in the Öresund region between Sweden and Denmark, which offers:

- A rich scientific environment with 11 universities, 10,000 researchers, and 165,000 undergraduate and 6000 postgraduate students;
- An excellent research infrastructure, close to other leading facilities such as the synchrotron at Max-IV in Lund and the free-electron laser facility XFEL in Hamburg, which provide complementary analytical techniques;
- The presence of an international, English-speaking community;
- A broad research-based and innovation-focused industry that has given the world ink-jet printing, Bluetooth, Sony Ericsson and AstraZeneca;
- An attractive surrounding landscape, along with a cultural diversity and high standard of living;
- Excellent communication with Copenhagen airport.

FOREWORD

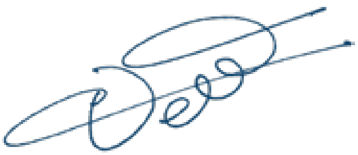


Advances in science and technology are strongly linked to the availability of state-of-the-art instrumentation and techniques for experiment and analysis, including all the methods that provide a detailed knowledge of the structure and the dynamics of matter at the atomic or molecular level. This is particularly true in the development of advanced materials.

Neutron and X-ray methods are essential – and complementary – tools in studying materials: X-rays probe the electronic clouds of atoms; while neutrons pinpoint the positions and motions of the nuclei, as well as giving information on magnetism at the atomic length-scale. Neutrons play a crucial role in elucidating information such as local structural arrangements and dynamics, as well as deformations, diffusion and quantum properties. In particular, in the field of organic chemistry, the precise location of specific hydrogen atoms is critical to understanding the biological function. Their positions can be established by substituting them with atoms of the heavier hydrogen isotope, deuterium. Indeed, neutrons – with their unique properties – offer a wide palette of scattering methods.

Neutron techniques are successfully exploited in many fields of materials research: in developing materials to improve the efficiency of energy use, in environmental technologies, in transport, and in manufacturing processes. They are a key tool in designing smart electronic components, functional nano-materials and novel biomaterials. Today, the evolution of technology calls for increasingly faster, more accurate and higher-resolution investigations of materials and components. The 'neutron tools' available must fulfil the needs of engineers and scientists, and match their future expectations. The European Spallation Source (ESS), to be built in Sweden, will deliver the bright neutron beams and innovative instruments that the user-community needs.

We at ESS feel that it is our role to ensure that scientists and engineers can benefit from the appropriate neutron methods and tools in their research.



Christian Vettier
DEPUTY DIRECTOR FOR SCIENCE, ESS

CONTENTS

INSIDE MODERN MATERIALS

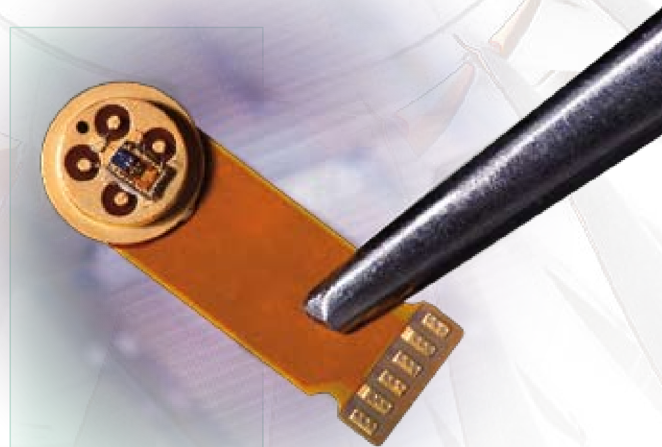
Axel Steuwer

Neutrons are an essential experimental tool in developing the materials of the future

Human progress is often defined by the materials developed and used in a specific era – from the prehistoric Bronze Age and Iron Age to the modern Silicon Age. Indeed, today, we live in a multi-materials world, which could equally be described as the Plastic Age or Liquid-Crystal Age – or even the 'Tetra-Pak' Age (referring to the well-known Swedish food-packaging system based on composite layered materials). Such materials, which are designed for a specific function, are pervasive in daily life, but often go unnoticed. Indeed, many consumer items such as mobile phones, cameras and spectacles contain a wide variety of different sophisticated functional and structural materials that most people are unaware of.

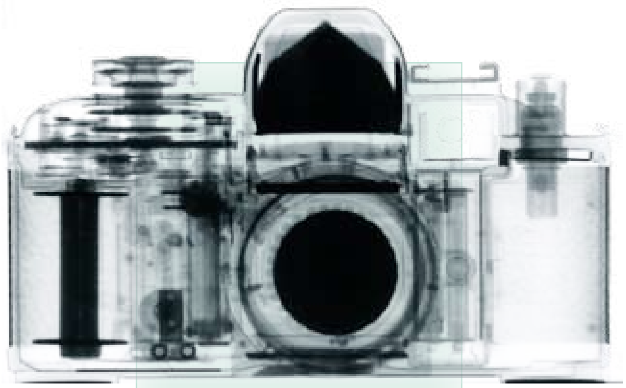
"Inventing is a combination of brains and materials. The more brains you use, the less material you need."
Charles F. Kettering
American inventor and head of research for General Motors (1920-1947)

Materials development is the cornerstone of technological advance – and therefore sustainable growth and economic competitiveness. The main driving forces are cost, performance, miniaturisation and, increasingly, environmental concerns. We need many kinds of new materials: biocompatible and biomimetic materials for medical implants and dentistry; improved catalysts for energy-generating devices such as fuel cells; lighter, stronger materials for aircraft; more environmentally-friendly, biodegradable detergents and packaging materials; and smaller, energy-saving devices for processing and storing information. The list of challenges for improved materials is virtually endless and spans all economic sectors. The total value of the materials-related market worldwide is in the tens of billions of dollars. Furthermore, the development of novel materials such as new high-temperature superconductors still has the potential to revolutionise our lives, in the same way as the iron axe or the transistor once did.


An Intel silicon chip

While some materials, such as Teflon (polytetrafluoroethylene) – often used to provide a non-stick coating – were discovered accidentally, today's materials are usually the outcome of clever innovation, combined with years of expensive systematic research and testing in order to optimise the desired properties. Increasingly, developments involve materials with a complex structure and function on ever-smaller scales; conventional laboratory equipment is often not sufficient to unravel the complexity, or to reveal how a material performs in real situations. A different set of tools is required, and neutron scattering is such a tool; it is unique in that it allows experiments to be undertaken in real, sometimes extreme conditions, while at the same time providing accurate information about processes down to the scale of atoms or molecules.

In this brochure, we showcase research across a wide spectrum of science and engineering fields, where neutrons provide unique and often critical insights into materials.

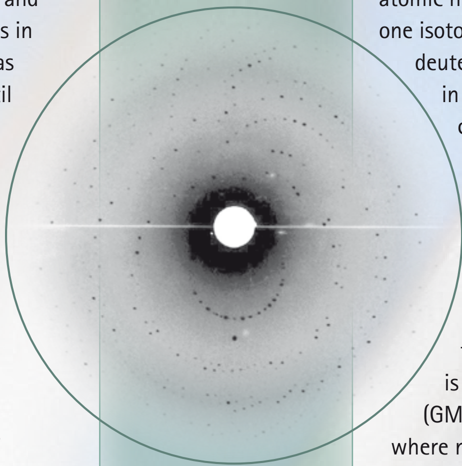

Neutron Imaging and Activation Group / Paul Scherrer Institute

Neutrons are highly penetrating and can 'see' inside objects (p.18)

WHY NEUTRONS?

Materials are made from assemblies of atoms, mostly chemically bound into molecules. They are sometimes arranged in an ordered, crystalline fashion and sometimes in a disorderly state as in glasses and liquids. They may form long intertwined chains as in polymers, or combine in complex arrangements as in proteins, for example. However, it was not until the discovery of X-rays, and then neutrons, in the first half of the 20th century that scientists could study the structure and behaviour of such structures at the atomic level.

X-rays can penetrate materials and are then scattered by the electron clouds of constituent atoms to produce a characteristic pattern of intensities. Beams of neutrons – particles composing the atomic nucleus, along with protons – are penetrating and behave like waves, which are also scattered by the nuclei of atoms. The distinctive fingerprints obtained from such interactions allow scientists to gather both structural (p.8) and dynamic (p.10) information. What makes neutrons a particularly versatile tool is that their wavelength can be easily tuned to match the scale being investigated – from tenths of a nanometre in common crystals to hundreds of nanometres in polymers (p.15) or biological structures.



A 2D Laue diffraction pattern

Another important characteristic is that the way in which neutrons are scattered depends on the types of atomic nuclei in the material. By selectively substituting one isotope of an element for another – such as deuterium for hydrogen – in different locations in the sample, specific structural components can be highlighted. Selective deuteration is a particularly important tool in studies of organic and biological materials (p.16).

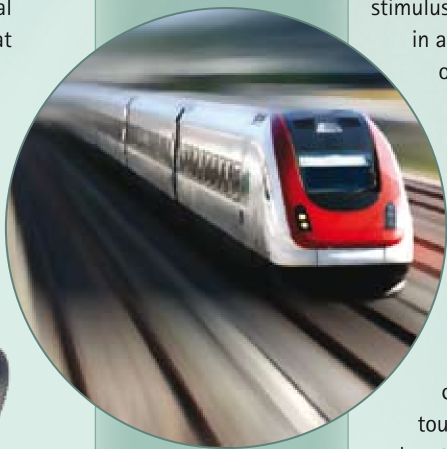
Neutrons also have a magnetic moment, so provide unique insights into magnetic and electronic materials, resolving their structures better than almost any other technique (p.13). A famous recent example is the discovery of giant magneto-resistance (GMR) used in computer hard-drive technology, where neutrons contributed towards unravelling the associated magnetic structure, which led to the award of the Nobel Prize for Physics.

Neutrons therefore represent an extremely versatile tool, providing many different kinds of information for diverse materials, over a wide range of scales, and under all kinds of conditions.

TYPICAL APPLICATIONS OF MATERIALS-SCIENCE RESEARCH

POWER TRANSMISSION

Superconductors can carry large amounts of electric current without loss but only at rather impractical low temperatures. Neutron diffraction has been at the forefront of research into superconductivity, paving the way for new materials that are superconducting at normal temperatures.



SMART MATERIALS

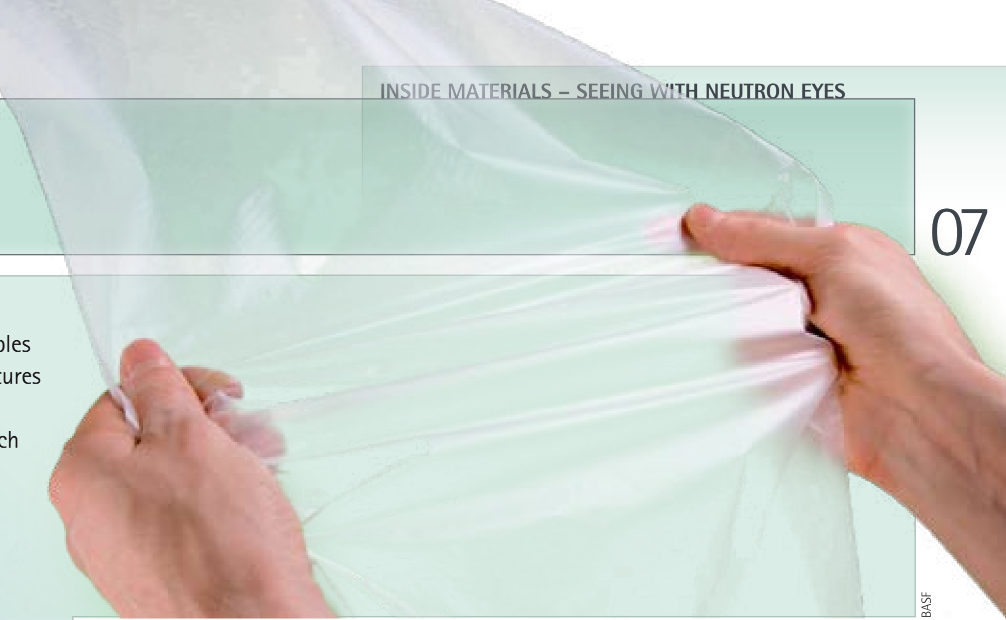
Smart materials are those that respond to an external stimulus such as stress, temperature or an electric field in a highly controllable way. They are often the basis of sensors and actuators. Neutrons can help in the design and fabrication of such materials, by uncovering how the induced changes in 'bulk' properties relate to what is happening to the arrangement of the constituent atoms.

ENGINEERING

Stresses in a material play a critical role in determining the lifetime of an engineering component and failure mechanisms. They can be beneficial when compressive – as in toughened glass for car-windshields, or detrimental when tensile – as around welds. Neutrons offer the only tool that can tell engineers about the stresses in a material without cutting it (p.17).

Self-healing polymer-coated nanoparticles for 'smart' scratch-resistant paint

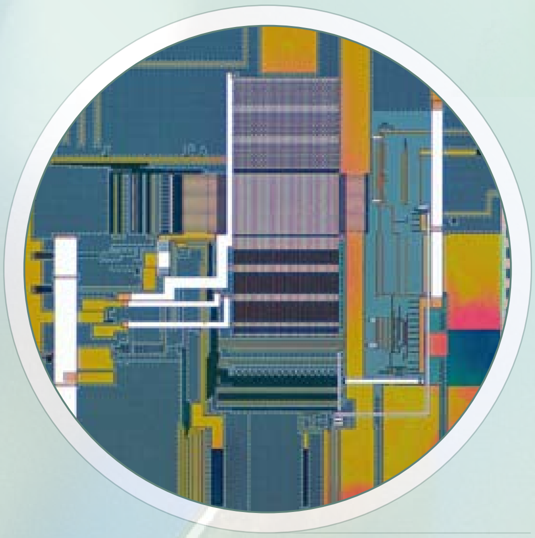
www.stefanfon.eu



BASF

SOFT AND BIOLOGICAL MATERIALS

Detergents, plastics and living tissue are all examples of soft materials which have complex, large structures made of elements that lend themselves to study with neutrons. They also contain hydrogen to which neutrons are particularly sensitive.



IBM

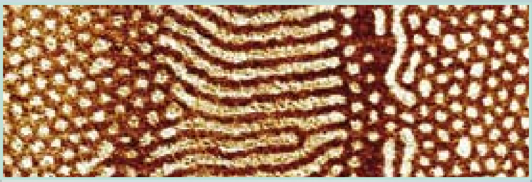
A magnetic memory chip

INFORMATION STORAGE

The next generation of computer memories and other devices will be based on novel magnetic materials. Neutrons provide a unique and sensitive probe of their magnetic structure and behaviour.

ENERGY GENERATION

Fuel cells (p.14) and the hydrogen economy are promising candidates as 'green' sources of energy. Because of their unique sensitivity to hydrogen, neutrons are being used extensively to study and optimise the chemical reactions that result in electricity generation, as well as to improve the overall design of water flow in these cells.



www.stefanbon.eu

A hybrid polymer nano-structure

NANO-MATERIALS

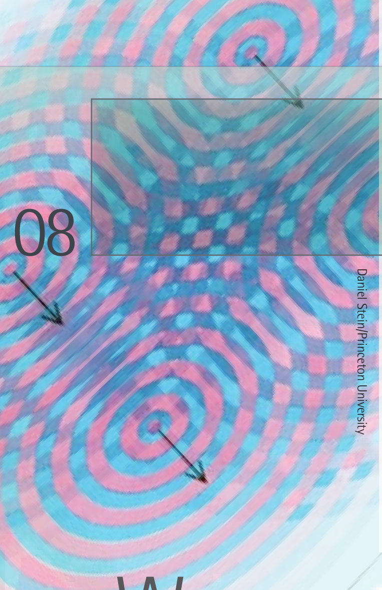
Nano-materials are structured on the scale of a nanometre (one-billionth of a metre). Simply by virtue of their size, nano-structures offer new electronic, magnetic or chemical properties, or improved performance as found in high-strength steels composed of, or containing, nano-sized particles. Studying these tiny structures with laboratory techniques is not easy, but is straightforward using neutrons (p.12).

WHY WE NEED A EUROPEAN SPALLATION SOURCE

Neutron beams for scattering experiments are typically produced in two ways: either with a nuclear reactor, or by using an accelerator system to generate high-energy protons, which then knock out neutrons from a target (a so-called spallation process). Currently, Europe has several national and international neutron facilities. Scientists at these institutes have led the way in neutron instrumentation and science, as well as in demonstrating the power of neutron techniques as tools to investigate microscopic structure in all kinds of materials, from exotic magnetic alloys to soft biological matter. To build on this success – and given the advancing age of existing neutron facilities – European countries are planning to build a new, more powerful neutron-scattering facility, the ESS, with a view to creating neutron instruments that are faster, more powerful and more accurate than those currently operating. The ESS will be the world's leading neutron source for many decades to come, and will enable the investigation of a wide range of materials in ever-more challenging environments. We are convinced that scientists will grasp this opportunity to perform their increasingly demanding experiments.

ZSW

Dr A. Steuwer is Visiting Professor for Materials Engineering at the University of Lund where he works for the ESS Scandinavia Secretariat.



Daniel Stein/Princeton University

EXPLORING INNER SPACE

Bob Cywinski

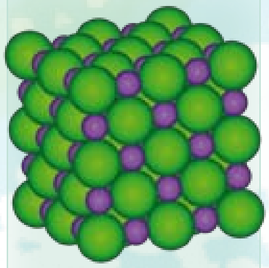
Neutrons offer a unique way of determining the structure of materials at the atomic and molecular level

When a beam of neutrons is scattered by the atoms in a sample, the neutron waves overlap and interfere with one other, like the ripples on the surface of pond, in a process known as *diffraction*. Measuring the intensity of the scattered beam at all angles then reveals how the neutrons have been influenced by the atoms in the material, and therefore what kind of atoms are present and where they are located.

BEAUTIFUL CRYSTALS

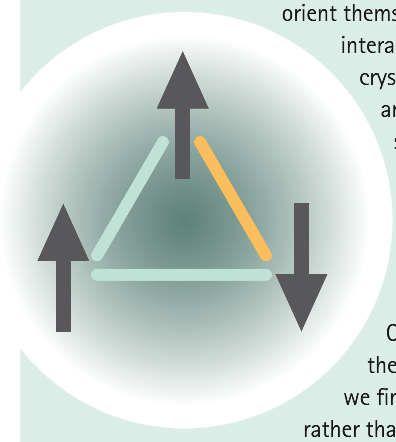
The images of the atomic positions and crystal structures are outstanding in their detail and exquisite beauty. The most commonplace of materials such as table salt or stainless steel appear as complex organisations of the constituent atoms, in which characteristic structural motifs are repeated in space to form a crystal lattice of precise symmetry. Moreover, even slight deviations from this perfect long-range order, such as those resulting from internal stress or strain in engineering components (p.17) – or from the substitution of a different atom or the lack of an atom in the crystal lattice – can be observed and studied. In this way, scientists can explore how changing the composition of a material affects its bulk properties and function.

Materials where the atoms are randomly arranged, as in a liquid or glass, can also be studied with neutrons. The sharp peaks associated with the diffraction pattern of a crystalline material are replaced by a smoothly varying distribution of scattered-neutron intensities, which provides information only on the probability of finding a particular atom at a particular position.



The crystal structure of sodium chloride

MATERIALS IN A SPIN



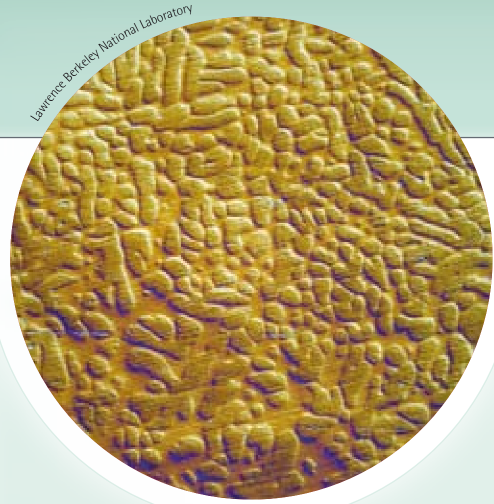
Theories of magnetic disorder predict how magnetic spins orient themselves in the presence of so-called frustrated interactions. For example, take a two-dimensional crystal plane in which the magnetic atoms are arranged on a triangular lattice. If every spin tells its neighbours, via the magnetic interaction, to point in the opposite direction to itself, how can the spins on a triangular lattice satisfy this demand? Using neutron diffraction, we now know they cannot – the result is instead a disordered 'spin-glass' state. On the other hand, in three dimensions, where the spins are arranged on a tetrahedral lattice, we find that a different situation pertains. Here, rather than forming a spin-glass state, the spins adopt an orientation that is similar to the orientation of the hydrogen bonds in frozen water – and so is called a 'spin-ice state'.

EXOTIC MAGNETISM

Neutrons have a magnetic moment or spin, which makes them a uniquely powerful probe of the magnetic fields associated with the electron spins in magnetic materials. Using beams of neutrons with spins all aligned, we can determine not only the magnitude of these magnetic spins, but also visualise how they are arranged in space and direction. Almost all of what we know and understand about ferromagnetic (spins aligned parallel) and antiferromagnetic materials (spins aligned antiparallel) comes from neutron studies.
Of great interest, currently, are exotic magnetic compounds with a more complex, spiral and helical, ordering of magnetic spins. Studies of these materials provide information for the development of novel electronic devices that employ electron spins for information storage and processing.

BIOLOGICAL STRUCTURES

An important advantage of neutrons is that they can resolve larger-scale molecular structures such as biological molecules and molecular assemblies, as well as polymers and nano-structured composites. The powerful technique of *small angle neutron scattering (SANS)* gives access to an extremely important field – that of 'soft matter' and biomaterials, which comprise many everyday products – from foods and medicines to plastic packaging and household furnishings. Increasingly, biologically-inspired materials with complex nanostructures are being used as sensors, tissue replacements, and even as putative devices for energy generation and electronic processing. Neutron scattering also has the advantage that it can analyse the components of large organic structures in solution. These contain large amounts of hydrogen that can be replaced by its isotope deuterium – which has a different scattering strength. By selectively deuterating one component so that its scattering intensity matches that of the deuterated solvent, it can be rendered invisible, so that other components then stand out; this is called *contrast matching*.

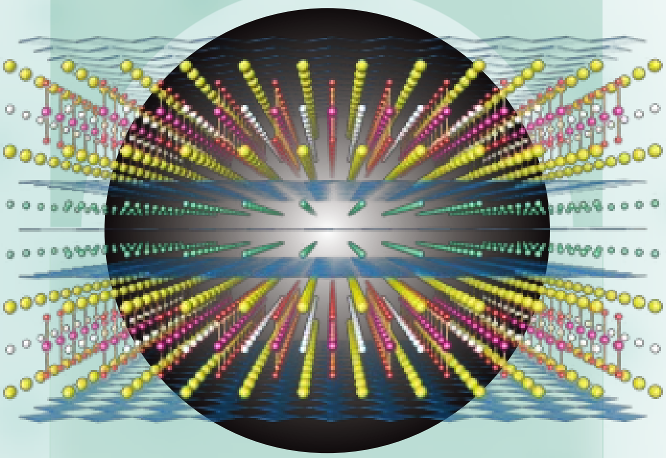


The micro-structure of a complex metallic glass

NEW SUPERCONDUCTORS

Neutron scattering has played a key role in studies of the famous copper-oxide ceramics that become superconducting (carry electricity without resistance) at temperatures above that of liquid nitrogen. The temperature at which these amazing properties appear can be tuned by changing the amount of oxygen within the crystal lattice, or by changing the chemical composition through substituting different metals. Neutron diffraction enables these changes to be observed and quantified, thereby providing information on which parts of the structure have the most effect on the superconducting properties.

P.P. Edwards and Martin Jones/University of Oxford



The layered structure of a high-temperature superconductor

TOUGH METALLIC GLASSES

A new class of materials can now be prepared by cooling molten alloys at the rate of millions of degrees a second, with the consequence that the atoms do not have sufficient time to reorganise themselves into a well-ordered crystal lattice. Such 'amorphous' alloys are strictly 'glasses', yet are structurally much stronger than their crystalline counterparts because they lack defects; normal metals are composed of crystalline grains, and the boundaries between the grains are a source of weakness. Metallic glasses are therefore extremely resistant to corrosion and wear. Neutron diffraction shows that although the atoms are still locally arranged in a well-defined motif, over longer distances these motifs are disordered, and the lengths of the bonds between the atoms can vary by several per cent. As a result, the long-range order is lost and the crystal lattice is no longer evident.

SURFACES AND THIN FILMS

Materials in the form of thin films are becoming increasingly important in many sectors including electronics, coatings and paints. Modern cleaning materials often have a complex nanostructure composed of thin layers of long-chain molecules such as detergents. A version of neutron scattering – *reflectometry* – in which neutrons are reflected off surfaces and interfaces – is becoming ever more important in studying thin films of commercial significance.

In all these studies, we are at present working close to the intensity and resolution limits of current facilities, yet experiments show that there is much more to be seen. Neutron scientists are waiting for the ESS to open a new and more powerful window into the intricacy and beauty of inner space.

ISIS/STFC Rutherford Appleton Laboratory

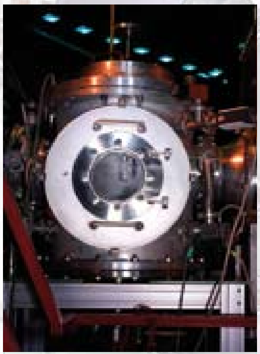
REFERENCES:
1. *Neutrons and new materials*: www.ill.eu/science-technology/science-at-ill/materials-science-engineering

Professor R. Cywinski is University Research Professor and Dean of Applied Sciences at the University of Huddersfield, UK.

THE LIFE AND TIMES OF MATERIALS

Margarita Russina

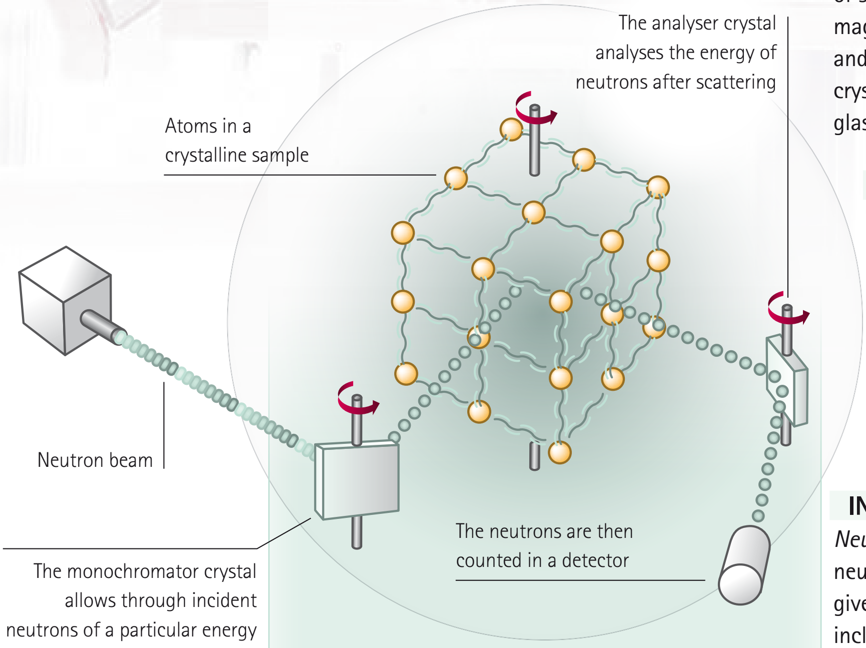
Uncovering how the building blocks comprising a material move and change at the microscopic level is the key to understanding its properties



The BRISP time-of-flight spectrometer at the Institut Laue-Langevin (ILL) in Grenoble, France

The development of novel nano-structured materials and miniature devices depends upon gaining insights into the interplay between the dynamics and structure at the smallest scales. Neutron-scattering techniques can provide information about both aspects simultaneously, over a wide range of length and time-scales not accessible by other techniques. A further advantage of neutron scattering is that it can explore the cooperative motion of a group of particles, as in a liquid for example. It is, therefore, a crucial tool in modern materials research.

As described on p.8, neutron diffraction provides unique information about the structure of many materials by measuring the change in direction of the scattered neutrons and ignoring any changes in their energies. To study dynamical phenomena such as the motion of atoms and molecules, or magnetic changes, requires that the neutrons exchange energy with them – this is called *inelastic scattering*. The resulting change in neutron energy, as measured by the change in their velocities in the scattering, then provides information about the motion of the particles in the sample. Inelastic scattering results can be displayed as spectra, so that the technique is often called *neutron spectroscopy*. Neutron spectroscopic methods can be divided in four types as described opposite.



A TRIPLE-AXIS INSTRUMENT LAYOUT FOR INELASTIC SCATTERING
The monchromator and analyser crystals, and sample can all be rotated. When neutrons interact with the sample, they cause the atoms or their magnetic spins to oscillate. The resulting energy loss or gain in the scattered neutrons gives information about the atomic or magnetic dynamics in the sample

FAST CHANGES ON THE FEMTO-SCALE

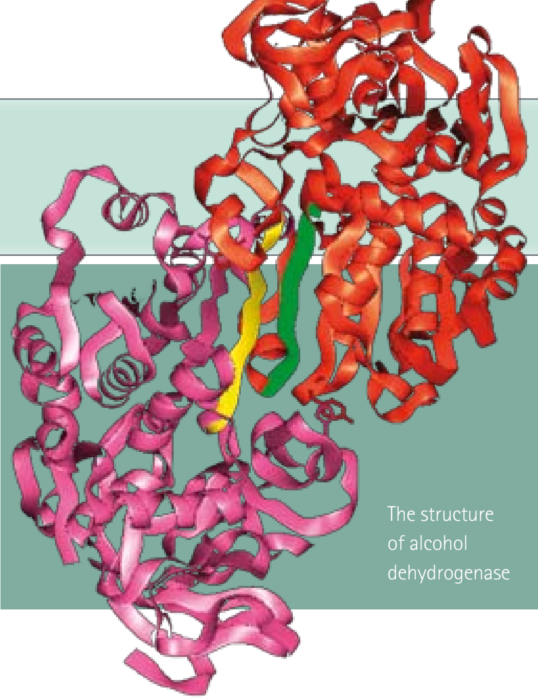
The first type encompasses *triple-axis and time-of-flight (TOF) spectroscopy*, which covers dynamic changes happening between a femtosecond and one-tenth of a nanosecond (10^{-15}–10^{-10}s). A triple-axis spectrometer, first developed in the 1950s, can directly measure the scattering energy in selected directions, while a TOF spectrometer measures the direction and velocity of the neutrons after the scattering. They are then converted into energy readings as a function of the scattering angle. Applications cover a broad field including high-frequency vibrational spectroscopy used to characterise molecular bonds in materials, the electronic behaviour of superconductors, magnetic excitations in molecular magnets, magnetic quantum fluctuations in thin films and layered materials, local and collective vibrations in crystalline and amorphous materials, and fast flow in glasses and melts.

NANOSECOND MOTION

Neutron backscattering, in which the energies of neutrons are analysed by nearly-backward scattering on analyser crystal arrays, allows dynamics to be measured over the nanosecond time-scale (10^{-10}–10^{-9}s). This is useful for studying changes in the orientations of molecules, so-called quantum tunnelling excitations, and dynamics in biological systems and viscous liquids.

IN THE SLOW LANE

Neutron spin echo (NSE), which uses the spins of neutrons as a marker to observe their velocity changes, gives access to motions across a broad dynamic range, including very low-energy processes happening over the microsecond scale. It is routinely used to study the slower motions associated with large molecular components such as proteins and polymers (p.15), as well as glasses and supercooled liquids. A recent development is the combination of triple-axis and NSE spectroscopy to study the lifetimes of excited quantum states in magnetic materials.



Birkbeck, University of London/Crystallography

The structure of alcohol dehydrogenase

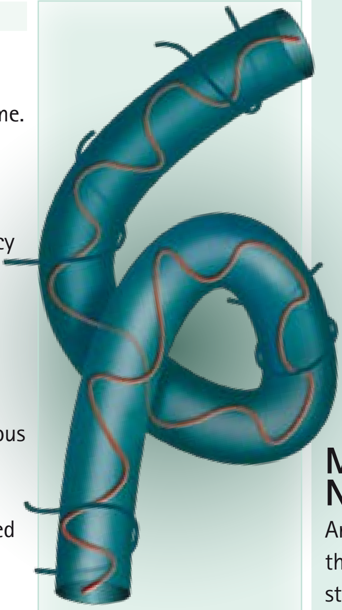
NANO-MACHINES AT WORK

The NSE investigation of the motions of large domains in protein molecules is crucial for the understanding of their behaviour as 'nano-machines'. A recent study of the protein, alcohol dehydrogenase, the enzyme responsible for breaking down alcohol in the body, helped to identify how the protein interacts with the substrate molecule. The protein consists of two identical sub-units. When the exterior domain binds to the substrate, it tilts outwards and opens the cleft containing the active site where the substrate reacts, while the inner domain between the monomers remains stiff. This opening motion provides the configurational freedom needed for biological function.

EVEN SLOWER ....

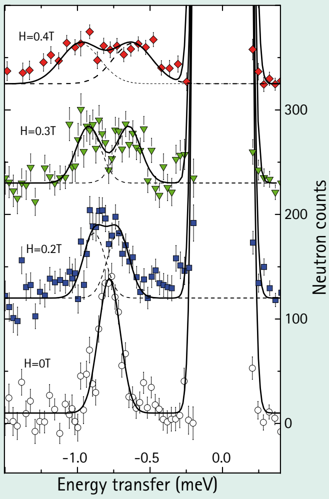
Real-time experiments represent the fourth emerging group of techniques, which consist of observing the change in counting rate of scattered neutrons over time. Correlation methods, such as the new time-resolved small angle neutron scattering technique, *TISANE* – in which the frequency of an instrument called a beam chopper is synchronised with the modulation frequency of a particular state in a sample – offer access to a time-range spanning micro- and milliseconds. The TISANE method has been successfully employed to study the relaxation of magnetisation in magnetic nanoparticles in ferrofluids.

These techniques, originally developed for continuous neutron sources, can be efficiently adapted to pulsed sources such as the ESS. New techniques being developed, combined with the higher intensity provided by the ESS, open up the way to unprecedented new capabilities for spectroscopy, with a range of neutron energies, in the coming years.



Polymers consist of long chain molecules that appear to move slowly within a tube-like volume. Neutron spin echo can analyse these movements

The ILL's neutron spin echo spectrometer, IN11



Inelastic neutron-scattering measurements taken over a range of magnetic field strengths (H) at just above absolute zero reveal the intriguing magnetic behaviour of lanthanum strontium cobaltite

MEASURING MAGNETIC NANO-CLUSTERS

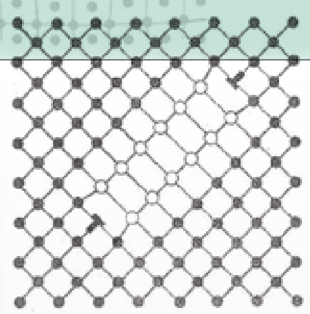
An example of the application of TOF spectroscopy is the recent study of the magnetic mineral lanthanum strontium cobaltite, $La_{1-x}Sr_xCoO_3$ – a naturally-occurring analogue of artificial nano-magnetic materials. It consists of magnetic nano-clusters, between 2 and 3 nanometres across, embedded in a non-magnetic matrix. Slight variations in the proportion of strontium strongly affect the magnetic interactions both inside and between the clusters, leading to dramatic variations in magnetisation and its temperature dependence. Recent inelastic neutron-scattering results on $La_{0.998}Sr_{0.002}CoO_3$ shed light on this controversial behaviour. At a temperature just above absolute zero (1.5K), the inelastic spectrum revealed a well-pronounced feature which is absent in pure lanthanum cobaltite. This signal is strongly dependent on the magnetic field, indicating an unusually high magnetic moment resulting from the presence of magnetic clusters of several cobalt ions. The data also suggest that the magnetic moment is actually dynamically spread over the whole octahedrally-shaped cluster.

REFERENCES: **1.** F. Mezei, *Journal of Neutron Research*, 1997, **6**, 3.
2. A. Podlesnyk *et al.*, *Phys. Rev. Lett.*, 2008, **101**, 247603.
3. R. Biehl *et al.*, *Phys. Rev. Lett.*, 2008, **101**, 138102.

Dr M. Russina is a scientist at the Helmholtz Zentrum Berlin where she is responsible for the time-of-flight spectrometer NEAT.

THE HIDDEN STRENGTH OF SUPERALLOYS

Gernot Kostorz

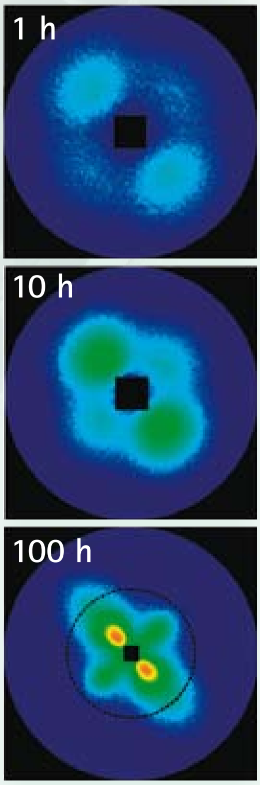


Examples of precipitates in superalloys

Neutrons uncover what makes some alloys super-strong even at high temperatures

Many properties of solid materials are sensitive to both the arrangement of individual atoms or molecules and their agglomeration on the scale of nanometres and micrometres. This is true for alloys, which may form homogeneous solid solutions of metal atoms at high temperatures, but upon cooling start to separate into new phases with different structures; small particles of one crystalline phase may precipitate within the matrix of another. This process is extremely important in the age-hardening of structural alloys, as the precipitates strengthen the alloy by hindering the plastic (irreversible) deformation of the matrix, which happens by local shear (slip) processes. The carriers of these shear processes are called dislocations. The effectiveness of age-hardening depends upon the size and distribution of precipitates attained in the early stages of phase separation.

Because the dimensions of the particles and the distances between them are in the nanometre range, this process and its consequences can be probed by small-angle neutron scattering (SANS). The method is particularly suited to following structural changes in such alloys, which show only low absorption of neutrons and good scattering contrast, giving high sensitivity and experimental precision.



SANS patterns of a nickel-titanium crystal at 870K as it ages over 100 hours

ORDER OUT OF CHAOS

Nickel-base alloys are widely used in structural applications such as gas-turbine blades, because of their strength at high temperatures and resistance to corrosion. The high-temperature performance of these 'superalloys' is due largely to the presence of crystalline precipitates in the matrix. The precipitated particles have a more ordered structure than the surrounding matrix and offer strong obstacles to the movement of dislocations. Frequently, there is also a misfit between the cubic crystal lattices of the particles and the matrix, which additionally serves to inhibit dislocation motion.

Some years ago, we used SANS to study the nano-structure of nickel-rich alloys containing titanium. For example, we took SANS patterns of a single crystal of a nickel-titanium alloy as it aged, *in situ*, in the neutron beam at 870K. The average diameter of the particles forming at this temperature, after being cooled rapidly from higher temperatures, increased from about 6 nanometres after 10 hours to about 14 nanometres after 100 hours of ageing. We noted that they lined up strongly in directions in which there was more 'give' in the matrix.

In-situ SANS was also used to study the formation of the most stable phase of this alloy, the *eta* structure, which has a chance to grow only if the alloy is kept at sufficiently high temperatures. Unexpectedly, when the homogeneous alloy was cooled from 1440 to 1200K and kept there, the SANS measurements showed that the nanometre-sized cubic particles still precipitated initially, before being overtaken by the progressive growth of the larger thin platelets of the *eta* phase.

These and other neutron-scattering studies can reveal changes over a wide range of distances within a complex metallic material with remarkable sensitivity. This helps in constructing and testing computer models of how atoms arrange themselves in alloys, and thus leads to a better understanding of their performance under real-life operating conditions. The work is expanding and covers more complex cases, which include more technologically relevant alloys.

Rolls Royce

REFERENCES: 1. G. Kostorz, *Z. Kristallog*, 2003, **218**, 154.
2. G. Kostorz and B. Schönfeld, *Chimia*, 2001, **55**, 517.

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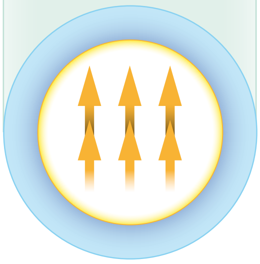
AND NOW, THE TERABYTE TAPE CASSETTE

Kazuhisa Kakurai

Polarised neutrons reveal the magnetic properties of novel nanoparticles for ultra-high-density data storage

Despite advances in the development of hard-disk memories, magnetic tape is still indispensable for storing the huge amount of audio and video data communicated via the broadcasting media, as well as for high-capacity computer back-up systems. Magnetic tape is both reliable and cost-effective. To date, the maximum capacity of a magnetic-tape cartridge is 800 gigabytes. However, the ever-increasing amounts of electronic data generated suggest that even higher data-storage capacities are required – into the terabyte (1000 gigabyte) regime.

The structure of the $Fe_{16}N_2$ nanoparticle showing the non-magnetic surface layer and magnetic core



Information is stored on magnetic tape as magnetic particles, originally of ferric oxide. A larger capacity requires increasing both the density of recording tracks on a tape and also the density of particles on each track. To realise these goals, the particles need to be as small as possible, while retaining a large saturation magnetisation (high total magnetic moment) and high coercivity (magnetic field strength needed to change the magnetisation). Most magnetic tapes employ needle-like particles; however, to reach higher densities, nano-scale spherical particles are essential. The ideal material should also be a cheap, iron-based compound that is chemically stable.

After a great deal of research, an iron-nitride cluster compound $Fe_{16}N_2$ was found to fulfil most of the requirements. This is a well-known material, once well-studied because of its possible giant magnetic moment (a result of adding up all the magnetic moments of 16 iron atoms in the atomic cluster). The giant magnetic moment in $Fe_{16}N_2$ is still controversial because this material phase is only quasi-stable and strongly oxidisable. To overcome this problem, one of the leading companies making magnetic tapes, Hitachi Maxell, developed $Fe_{16}N_2$ nano-particles coated with a protective surface layer – called NanoCAP (nano-composite advanced particles). The company has succeeded in synthesising coated particles with an average overall diameter of only 16 nanometres, and is currently developing a method of mass-producing terabyte-class magnetic-tape cartridges.

An electron micrograph of $Fe_{16}N_2$ nanoparticles

INSIDE MAGNETIC NANOPARTICLES

To achieve yet higher densities requires particles with an even smaller average diameter. A detailed knowledge of the magnetic moment of the $Fe_{16}N_2$ core and its dependence on size, as well as its average structure, is thus highly desirable. However, measurement of the bulk magnetisation cannot reliably determine the core's magnetic moment because of uncertainties regarding the thickness of the non-magnetic coating. Electron microscopy seems to give a contrast picture indicating the core structure, but it does not necessarily reflect the non-magnetic/magnetic core structure.

Neutrons have a magnetic moment, and diffraction experiments using beams of polarised neutrons (all magnetic moments pointing in the same direction) are now an established way of analysing the magnetic structure of materials at the nanoscale. We carried out both polarised-neutron powder diffraction, and small-angle magnetic scattering to access directly the magnetic moment and structure of the $Fe_{16}N_2$ core. We found that the averaged magnetic moment of the iron atoms in $Fe_{16}N_2$ nanoparticles to be comparable to that of crystalline iron, and the magnetic core diameter to be 11 nanometres. It is clear that these polarised neutron measurements will contribute to the development of high-quality magnetic nano-particles for the even higher density magnetic-tape storage media that will be needed in the future.

REFERENCES: **1.** Y. Sasaki *et al.*, *IEEE Trans. MAG.*, 2005, **41**, 3141.
2. M. Takeda *et al.*, *Nucl. Instrum. Methods, Phys. Res. A*, 2008, **586**, 229.

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OPTIMISING PROCESSES IN FUEL CELLS

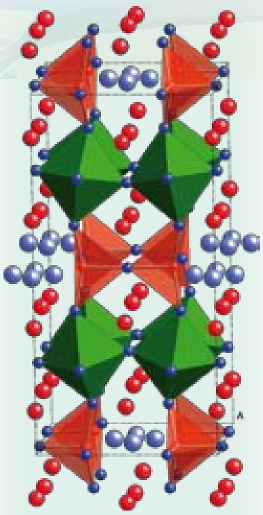
Gunnar Svensson

Neutron diffraction is an essential technique in the hunt for new materials for electricity generation

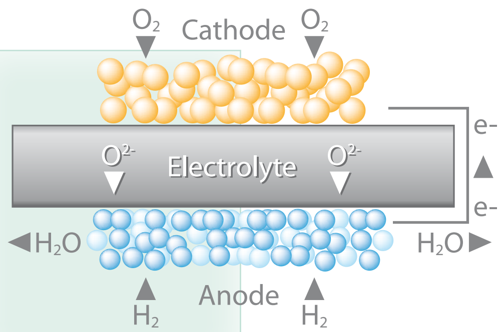
Growing environmental problems and energy use are major issues for the whole world. We need to improve the production of high-quality energy like electricity from both non-fossil and fossil-based fuels, while at the same time decreasing carbon-dioxide (CO_2) emissions. One contribution will be fuel cells. Their attraction is that they directly convert chemical energy to electricity with the minimum of dangerous exhausts, and with efficiencies ranging from 40 to 80 per cent depending on type. In principle, only water is formed if the fuel is hydrogen – together with CO_2 if hydrocarbons are used.

A practical fuel cell consists of a stack of units, each containing a catalytic anode and cathode separated by an electrolyte. The electricity is produced by oxidising hydrogen at the anode, forming protons (H^+) and electrons. Electricity becomes available as the electrons pass through the external circuit back to the cathode. There, they reduce oxygen (O_2) from the air to oxide ions (O^{2-}), which react with protons from the anode to form water.

Today, there are several kinds of prototype fuel cells with operating temperatures varying from slightly above room temperature up to 1000°C. Solid-oxide fuel cells (SOFCs), which have ceramic electrodes and electrolytes, have a much higher flexibility in the type of fuel used because of their high operating temperature of 750 to 1000°C. One electrolyte used in SOFCs is yttrium-stabilised zirconia (ZrO_2), which conducts the oxide ions to the anode. The high operating temperature, however, leads to mechanical problems resulting from the difference in thermal expansion properties of the ceramic materials involved. There is therefore a strong demand to find new materials that work at lower temperatures of between 500 and 600°C.



The crystal structure of the potential fuel-cell material strontium yttrium cobalt oxide, $Sr_{1-x}Y_xCoO_{2.625-d}$



A typical fuel cell

NEW MATERIALS

Neutron studies are crucial for the structural understanding of new materials. The unique sensitivity of neutron scattering to light elements such as oxygen and hydrogen (deuterium), and to magnetic structures, makes it a powerful technique. Recent examples include high-temperature neutron-diffraction studies of candidate mixed oxides – $La_{1.54}Sr_{0.46}Ga_3O_{7.27}$ and $La_{0.9}Sr_{0.1}Ga_{0.8}Mg_{0.2}O_{2.85}$, to determine the crystal structure and the path of the mobile oxide ions in the structure at operating temperatures.

Alternatives to oxide-conducting electrolytes are proton conductors in which the protons travel to the cathode. The smaller protons generate a higher conductivity, although there are problems with the chemical reactivity of these materials. Quasi-elastic neutron scattering, combined with theoretical modelling, gives information about the proton diffusion. One example is the study of proton migration in yttrium or scandium-doped barium zirconate.

Researchers are also trying improve the electrode materials so that they are both electron and ion conducting, are chemically robust, and with a thermal expansion that matches that of the electrolyte. For many years, we have been interested in cobalt oxides as potential cathode materials. Here, structural information from neutron diffraction has been invaluable. One compound of interest has been a strontium yttrium cobalt oxide, which has oxygen-deficient layers. The distribution of oxygen in the layers and the oxidation state of the cobalt atoms are very important for the magnetic and electronic transport properties of these materials. A minute change in oxygen composition causes the material to change from being a semiconducting antiferromagnetic compound to a metal-like conductor with a ferromagnetic structure.

It is clear that neutron-diffraction studies will enable the development of fuel cells with reasonable production costs, not only in characterising candidate materials but also in *in situ* studies of operating fuel cells.

REFERENCES:
1. X. Kuang *et al.*, *Nature Materials*, 2008, doi:10.1038/nmat2201.
2. M. Karlsson *et al*, *Solid State Ionics*, 2009, 180, 22.

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FANTASTIC PLASTIC

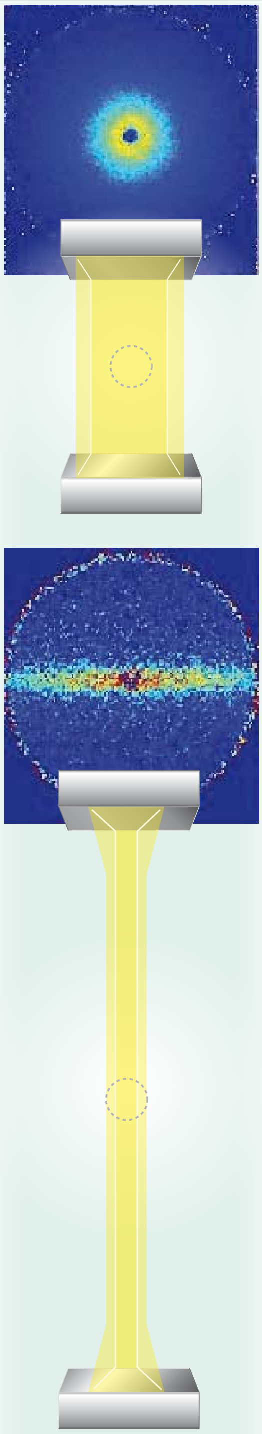
Kell Mortensen

Neutron-scattering techniques are the perfect tools for probing the complex structure and behaviour of advanced polymer materials

Polymers are large molecules, composed of hundreds or thousands of similar molecular components, linked together like pearls on a string, or in a network in more complex systems. They are found everywhere – as plastic packaging, rubber in tyres, textiles in clothes and furnishings, and in almost every kind of consumer item. All living systems contain complex bio-polymers. Increasingly, novel materials based on polymers, and nano-composites of polymers and inorganic particles, are being designed for specialised applications.

Because of their large dimensions, polymer chains are often highly entangled, like spaghetti. The result is that the materials demonstrate diverse structural and dynamic characteristics over a broad range of length and time-scales. On the short time-scale, typically seconds or less, an ensemble of polymers will behave like a solid with elastic characteristics. On longer time-scales, the material will flow like a liquid with low viscosity. This combination of solid and liquid-like characteristics is termed viscoelastic, and is attractive for many applications. An example is the rubber used in car tyres, where the combination of elastic properties at high frequencies efficiently transfers energy to motion, while the low-frequency viscous behaviour ensures the effective absorption of energy when the car is braking. The industrial processing of polymers also depends strongly on their flow properties, which are determined by the interactions and motions of the constituent structural units.

Neutron scattering is one of the main techniques employed to uncover the structure and dynamics of polymers over this wide range of length and time-scales. Small angle neutron scattering (SANS, p.8) can probe large-scale molecular structure, and the structural response of the macromolecules to shear strain and other deformations. Neutron spin echo (NSE, p.10) resolves how polymers move, while wide-angle neutron diffraction offers insights into the local inter- and intra-chain correlations, which are crucial, for example, in the formation of glassy structures in which the molecules are randomly arranged.



SANS experiments reveal how a polymer responds to stretching

POLYMERS TAKE THE STRAIN

Polymers are exposed to lots of strain and stresses during processing and applications. This sets major challenges for companies in manufacturing reliable, stable polymer products. Neutron-scattering experiments are crucial for understanding the origin of these problems, and they provide the basis for establishing parameters for optimal production. In a recent example, we studied the effect of shear on a tri-block copolymer gel (styrene-ethylene/butylene-styrene, SEBS). This is a strong, flexible material composed of blocks of polystyrene interspersed with blocks of poly(ethylene butylene). It is used as a medical plastic and also for electrical insulation. In an organic solvent, the polystyrene blocks curve round into nanoscopic balls or micelles, while the middle ethylene/butylene blocks form loops and bridges between the micelles, to create a network. The SANS studies showed how the material's texture changed depending on the rate and strength of the shear force applied, and that even at ambient temperatures the material is not purely elastic, but undergoes irreversible changes on both macroscopic and nanoscopic length-scales.

We also studied block copolymers based on polyalkylenes, which are among the best bio-compatible polymers, having low toxicity and immunogenicity. During their fabrication, however, significant amounts of impurities appear, which may affect their properties. Recent neutron-scattering experiments systematically explored how these impurities affect both the formation of the micelles and how they are arranged.

REFERENCES: 1. K. Mortensen *et al.*, *Macromolecules*, 2002, **35**, 7773. doi: 10.1021/ma0121013.
2. K. Mortensen, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2001, **183–185**, 277. doi: 10.1016/S0927-7757(01)00546-5.

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THE COMPLEX WORLD OF BIOMATERIALS

Giovanna Fragneto

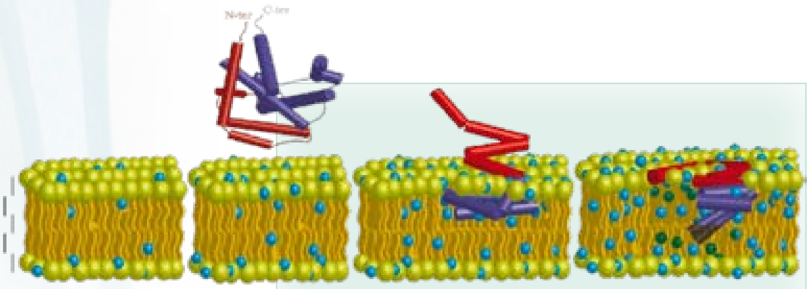
Investigating model membranes with neutrons provides an ideal way of understanding and designing new biomaterials

Biomaterials are materials used and adapted for medical applications such as joint replacements, artificial ligaments and tendons, dental implants, heart valves and contact lenses. They may be plastic, ceramic, metal or composite, or involve living cells grown on an artificial template. Of great significance is the interaction of proteins with these biomaterials – for example, proteins absorbed into polymer surfaces can cause fouling. Understanding how therapeutic proteins, or proteins from pathogenic microbes, interact with cell membranes is also crucial to treating disease, as well as in designing new bio-inspired nano-scale devices.

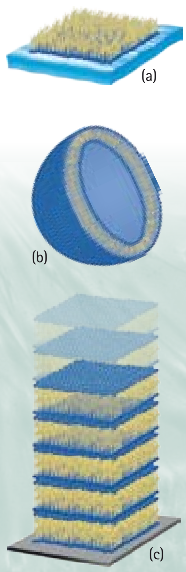
Physicists have been able to offer both structural and functional insights into these interactions through the study of model systems of biomaterials, such as polymers and cell membranes. The samples are prepared as thin, supported layers of lipids and other molecules such as proteins and cholesterol. These can then be patterned and manipulated in many ways to tune their architecture and physical properties for studies – ranging from exploring fundamental membrane-protein function to finding the optimum conditions for immobilising proteins for bio-sensing applications.

UNDERSTANDING MEMBRANES

Neutron scattering provides a unique set of analytical methods for studying model membranes. Neutrons are strongly scattered by the light atoms comprising soft and biological materials; they are also non-destructive and highly penetrating, so that buried and/or complex systems can be investigated. They give unique access to microscopic structure and dynamics at length-scales of intermolecular or atomic distances. The optimisation of instrumentation and sample-preparation techniques, as well as the new possibilities offered by protein deuteration (p.6), have opened the way to studies of lipid/protein interactions that were impossible in the past. We can now engineer systems that allow us to look at the insertion of biomolecules into membranes and to determine accurately the structure, as well as the dynamics of the interaction.



How the diphtheria toxin inserts into a cell



Model membrane systems probed by neutron scattering. They consist of layers of long-chain lipid molecules in various arrangements: (a) a monolayer at the air–water interface, (b) a small vesicle and (c) stacked bilayers

A recent example is the neutron study of how the diphtheria toxin inserts itself into a cell membrane. This small soluble protein is amongst the most studied bacterial molecules, and the mechanism by which it is released into a target cell is of interest to both biotechnologists and gene therapists. Materials pass into a cell via a membrane-bound compartment called an endosome, which has a higher acidity than the surrounding cell. However, the process is poorly understood, and in the case of the diphtheria toxin still controversial. The toxin has three domains including a translocation domain T, which is known to change shape at membrane boundary so as to initiate the structural and dynamic changes that then allow the catalytic domain to enter the cell.

We used neutron reflectivity to follow what happens as the T domain inserts into a model lipid membrane under increasingly acidic conditions that mimic those in a real cell. Contrast variation and partial deuterium labelling (p.8) of both the lipid bilayer and the toxin domain enabled us to gain unprecedented structural resolution of the phenomenon.

Biologists have started to appreciate the power of neutron techniques. The next generation of neutron-scattering instruments and sources will allow us to investigate the dynamics of proteins embedded in membranes in their natural environment.

REFERENCES:

1. G. Fragneto and M. Rheinstädter, *C. R. Physique* **8**, 2007, 865.

2. *A. Chenal et al.*, *J. Mol. Biol.*, 2009, **391**, 872.

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A BETTER AIRCRAFT WING

Lyndon Edwards and Axel Steuwer

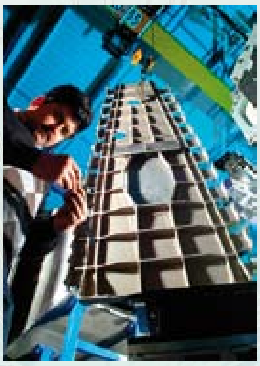
Neutron diffraction provides an excellent method for measuring residual stresses in critical engineering structures such as aerospace components

Most mechanical objects harbour residual stresses – invisible forces trapped within their structure at the atomic level – which are present even in the absence of external loads. The arrays of atoms in a metal, for example, may be pushed together in a compressive stress or pulled apart in a tensile stress. Almost every manufacturing process introduces such stresses, whether the constituent material is a metal, polymer, ceramic, or a composite. They affect the performance and lifetime of the component – but can be beneficial as well as detrimental. Pre-stressed concrete, tempered (safety) glass, and surface-treated metals are typical examples of materials, where incorporating beneficial stresses has improved their strength and durability. In each case, the processing is designed to generate – usually carefully balanced – compressive forces. Tensile stresses, on the other hand, tend to lead to more serious, detrimental effects, such as the premature failure of components due to cracking or deformation. An extreme example is the invisible tension in a balloon, which if pricked leads to spontaneous catastrophic failure, as the tension leads to very rapid propagation of the crack.

During the past two decades, neutron diffraction has established itself as a routine technique for probing residual stresses. It allows engineers to map stresses accurately in mainly metallic but also ceramic components, by measuring the tiny variations in inter-atomic distances in the crystal structure – which thus acts as an internal 'strain gauge'. The high penetration of neutrons enables measurements to be made non-destructively to depths of several centimetres in most engineering alloys.

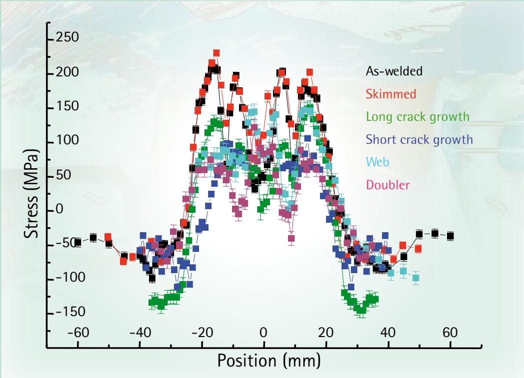
Neutron diffraction has thus become an important tool for engineering science, contributing significantly to the understanding of residual stresses in manufactured components, how they occur and how they can be mitigated. Diffraction measurements allow engineers to validate and compare computer models for predicting harmful stresses, and then devise treatments to limit them. The result is that virtually every neutron facility in the world, whether a reactor or a spallation source, hosts a dedicated beamline for materials engineering work. In fact, neutron-diffraction stress measurement is the only neutron-scattering technique for which an international standard has been laid down. A VAMAS (Versailles Agreement on Measurements and Standards) round-robin project established the reliability and accuracy of the method, and has led to the accreditation of an ISO pre-standard, which ensures that structural engineers can assess residual stresses with confidence.

STFC RAL/ISIS



Above: residual stress within aircraft wing welds being measured using the ENGIN-X instrument at the ISIS neutron facility in the UK

Right: residual stress profiles for the wing obtained during different stages in the manufacturing process



Institute of Materials Engineering/ANSTO

STRESSES IN WELDS

An interesting example is the mapping of stress profiles inside welds in aerospace materials. Welding is being considered as an alternative to rivets for joining structures such as aircraft-wing components. The process is cost-effective, saves on weight, and, if done correctly, should produce a more robust and durable join. Traditionally, residual stresses have been difficult to determine reliably and accurately in aerospace structures such as the wing-rib component being measured in the photograph above left. Stresses develop and evolve throughout the various production stages, and influence how cracks start and grow. They may then change as a consequence of in-service loading (such as take-offs and landings). These problems become particularly difficult when dealing with stresses arising from welding. The figure above shows the development of the residual-stress profile during the typical stages of manufacture of the wing component. These unique data allow engineers to compare critically the performance of welded wings with that of a traditional riveted construction.

REFERENCES:
1. P. J. Withers, *C. R. PHYSIQUE, 2007*, **8**, 806.
2. L. Edwards *et al.*, *Journal of ASTM International*, 2006, **3**, doi: 10.1520/JAI12547.

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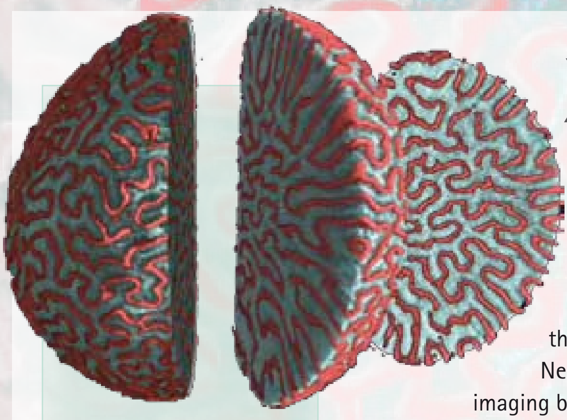
NEUTRONS GIVE THE BIG PICTURE

Eberhard Lehmann

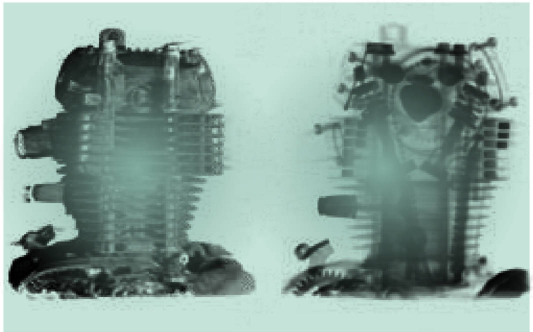
Neutrons can image the interiors of objects not readily accessed by X-rays



A stony coral (diameter about 10 centimetres) was studied with neutron tomography. The separation of hydrogenous zones is possible, and slices are made to show the inner distribution

X-rays provide a well-established way of seeing inside an object. They can reveal, through contrast, dense structures such as bone and teeth by the degree to which the X-rays are absorbed or scattered by their constituent heavy elements. Components consisting of light elements such as hydrogen, are transparent to X-rays. The resulting differential attenuation of the X-ray beam, after it has passed through a sample, is then detected – originally by film and now using digital detectors. Neutron beams can also be deployed in a similar manner to provide a two-dimensional neutron distribution; indeed, neutron radiography has been carried out since the 1940s, although the beam quality and the detection technique were then not very good.

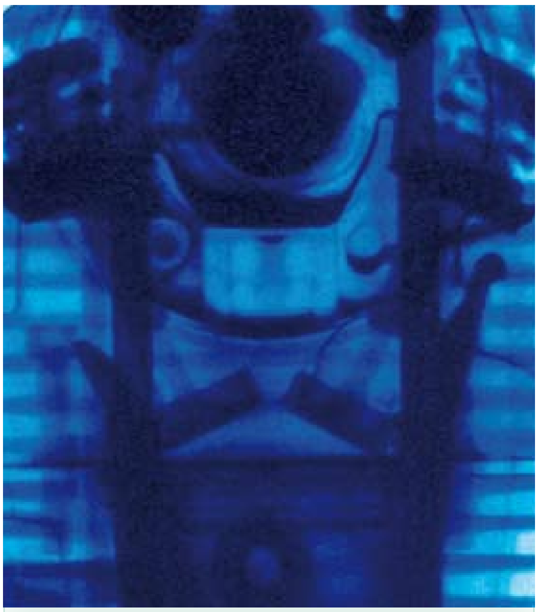
Neutrons are of interest for imaging because their transmission behaviour is different from that of X-rays, and so give complementary information. While X-rays are nearly ideal for examining the body because they pass through soft tissues containing a lot of hydrogen atoms – particularly in water, neutrons are extremely sensitive to hydrogen and cannot penetrate even a few centimetres of water. However, slow neutrons (therefore with low energies) can detect and visualise small amounts of hydrogenous material. This is especially useful if it is encapsulated within a heavy, compact structure that is not transparent to X-rays. Examples include water absorbed by porous stone, soil or wood, thin oil films in engines, or the adhesive joints between metal components.



The results of the tomography investigation of a combustion engine: left, the outer structure is shown; right, the cover is 'withdrawn' and inner components are visible

IMAGING REQUIREMENTS

Neutrons are not as readily available for transmission imaging as X-rays, being produced by the nuclear processes of fission, spallation or radioactive decay. The neutrons emitted are very fast, and to make them useful for materials research, they have to be slowed down to low energies. To give the optimum image quality and spatial resolution, the neutron beam also needs to be intense, uniform and well-collimated. Finally, the beam size, the detector area and the sample size have to fit together in the best possible way. It is no surprise, therefore, that there are not many facilities in the world that can optimally fulfil all these requirements. Furthermore, current facilities cannot easily accommodate neutron imaging alongside conventional neutron scattering.

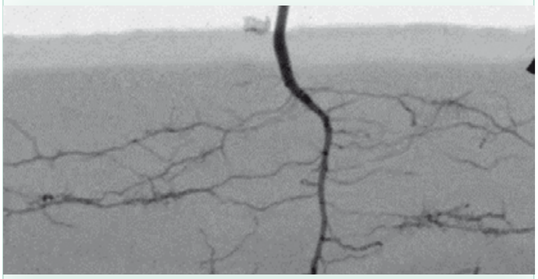


The same engine as above inspected over time, when running at 1000 rpm. The most interesting question was the change in the lubricant (oil) distribution during motion

NEW TECHNIQUES

Nevertheless, new neutron-imaging methods are now available, which are particularly useful for materials studies. Neutron tomography, whereby a series of image 'slices' through an object are combined to give a three-dimensional representation, is now a standard tool (similar to computer-aided X-ray tomography, or CAT). Neutron and X-ray studies can be performed simultaneously or sequentially with the same set-up, to provide complementary results.

Originally, film was used for neutron imaging; however, in the past few years, new digital detectors have been developed that allow the data to be acquired in seconds. With faster image acquisition, it becomes possible to make neutron 'movies' with high frame rates, either in real time, or by repeating an experiment and taking an image after a given time period. In addition to obtaining visual information based on attenuation – which corresponds to the material density and the strength of neutron interaction – the wave properties of neutrons can also be exploited to extract phase information as another source of data.



Living plants can be studied with respect to their root behaviour, because of the high contrast in organic material for neutrons. The moisture content of the surrounding soil structure can also be determined non-invasively

APPLICATIONS

Neutron radiography has applications in a wide variety of areas. A prominent recent example is in fuel-cell research. The most promising type of fuel cell electrochemically combines hydrogen and oxygen to generate electricity. Because the product is water, which dramatically affects the performance, detecting and visualising the water distribution in an operating cell is highly relevant. Such studies are in progress in several laboratories, in close collaboration with industrial partners.

The uptake of moisture in soil, wood and building materials can also be visualised and followed with neutrons in two or three dimensions. Even the growth of plant roots *in situ* can be investigated in relation to soil and moisture properties, and also contaminants.

Objects of cultural heritage have been studied successfully with neutrons. Because they can penetrate metals, corrosion and evidence of previous restoration can be detected. Neutron tomography allows a kind of virtual dissection to be carried out, revealing interior structures and thus information about the manufacturing process used.

The renaissance bronze from the Rijksmuseum in Amsterdam, sculpted by Johan Gregor van der Schardt in the 16th century, was investigated with neutron tomography. The images, from top to bottom, show the sculpture, a full neutron radiograph, and a single slice though the object

Neutron imaging can also be applied to some heavier materials. Both uranium in nuclear fuel and its cladding are transparent to neutrons. Because the two relevant isotopes uranium-235 and 238 show very different contrasts, enriched and burnt fuel can easily be studied with neutrons in a non-invasive way. Furthermore, since neutrons are also sensitive to hydrogen, embrittlement of the cladding caused by the absorption of hydrogen can also be detected.

FUTURE CHALLENGES

In the past few years, technical advances have resulted in improvements in the spatial resolution of neutron imaging so that it now starts to compete with those of X-ray and synchrotron radiation systems. A resolution of about 10 micrometres has been achieved, with scope for further improvement. However, to improve imaging further, much higher beam intensities are required.

Another challenge is to narrow the energy band of the initial beam, in particular in the lowest neutron-energy range. This would enhance, for example, any scattering signals from artefacts in crystalline structural materials, and would provide a new way of characterising the solidification process in welds and solders.

A high-intensity spallation pulsed neutron source would provide the requirements for such experiments. Pulses of neutrons with different initial energies, and therefore speeds – based on the time-of-flight principle, where the fast neutrons are detected earlier than the slower ones – can be used to perform energy-selective imaging studies to give more information. Neutron beam-lines for this purpose are under consideration, or are being developed, at facilities in the US, Japan and the UK. The ESS, to be built in Sweden, is a step in the right direction for advanced neutron imaging.

There are many other potential applications of neutron radiography. Improved imaging methods combined with dedicated imaging beam-lines, and supported by promotion across a wider range of disciplines, will secure a bright future for this challenging technique. Achieving these goals will ensure that neutron imaging advances in step with complementary X-ray methods.

REFERENCES: 1. E. H. Lehmann *et al.*, *Annual Report 2004*, Annex NUM, http://num.web.psi.ch/reports/2004/ASQ/asq-2004-48.pdf
2. F. Pfeiffer *et al.*, *Phys. Rev. Lett.*, 2006, **96**, 215505.

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GLOSSARY

ALLOY
A solid homogeneous mixture of two or more metals.

ANTIFERROMAGNETISM
A type of magnetic order in which the electron magnetic moments are alternately oppositely aligned.

BIOMATERIAL
A natural or man-made material used in components that are designed to interact with, or replace, living tissues or organs.

BLOCK COPOLYMER
A material consisting of alternating segments of more than one type of polymer.

CELL MEMBRANE
A double semi-permeable layer of lipids and other molecules, which surrounds all living cells and organelles in cells.

COERCIVITY
The magnetic field intensity needed to demagnetise a fully magnetised material.

CONTRAST MATCHING
A technique whereby a proportion of hydrogen atoms in a selected molecular component of a complex system, or its solvent, is substituted with deuterium, such that the scattering strength of the component matches that of the solvent, rendering the component invisible, and thus allowing other components to be seen more clearly.

CONTRAST VARIATION
A technique in which certain atoms in a sample are substituted by another isotope with a different scattering strength in a way that preferentially enhances the scattering pattern of particular components of interest.

CRYSTAL LATTICE
The regular three-dimensional array of atoms or molecules in a crystalline material.

DETERGENT
A cleaning material, usually based on surfactants – long-chain molecules that have both water-loving and oil-loving components.

DEUTERATION
The (chemical) replacement of a hydrogen atom in a molecule with its isotope deuterium.

DEUTERIUM
A heavier isotope of hydrogen having a neutron as well as a proton in the nucleus.

DISLOCATION
A defect, or irregularity, within a crystal structure, in which planes of atoms are bent or twisted.

ENZYME
A type of protein that mediates a specific chemical reaction in living systems.

FEMTOSECOND
One-million billionth (10^{-15}) of a second.

FERROFLUID
A material composed of magnetic nanoparticles suspended in a fluid.

FERROMAGNETISM
A type of magnetic order in which the electron magnetic moments are all aligned.

INELASTIC SCATTERING
A neutron technique in which there is an exchange of energy between the neutrons and the molecules being studied, thus giving information about their motion and flexibility. (When a neutron is scattered elastically, there is no energy transfer.)

ISOTOPE
A particular form of an element as defined by the number of neutrons in its nucleus. The isotopes of an element have different masses but similar chemical properties.

LIPID
A molecule consisting of a long hydrocarbon chain with an electrically charged group of atoms at one end. Lipids arrange themselves in layers and are the basis of biological membranes.

MAGNETIC CLUSTER
A group of several chemically linked atoms with magnetic moments that combine to give a giant magnetic moment.

MAGNETIC DIFFRACTION
An additional scattering phenomenon to normal diffraction (see Neutron diffraction), resulting from any magnetic properties of atoms in a structure.

MAGNETIC MOMENT
An effect arising from a spinning electric charge. Atoms have magnetic moments as a result of the spin and orbital motions of any unpaired electrons. Neutrons also have a magnetic moment.

METALLIC GLASS
A metallic material in which the atoms are randomly arranged rather than forming an ordered crystalline structure.

MICELLE
A cluster of small molecules such as lipids or surfactants that assemble together in a solution, often with distinctive arrangements depending on chemical composition.

NANOCOMPOSITE
A material composed of more than one compound organised at the nano-level.

NANOMACHINE
A nano-scale mechanical device.

NANOMETRE
One-billionth (10^{-9}) of a metre.

NANOSECOND
One-billionth (10^{-9}) of a second.

NANOPARTICLE
Particles of matter at the scale of nanometre. They often have specific properties connected with their size.

NANOSTRUCTURE
A structure designed at the nano-scale.

NANOTECHNOLOGY
The manipulation of materials and their physical and chemical properties at the scale of a nanometre.

NEUTRON
One of the two particles found in the atomic nucleus. They have a characteristic wavelength depending on energy.

NEUTRON BACKSCATTERING
A technique in which the energies of neutrons reflected backwards are measured. The energy of the backscattered neutrons is precise enough to allow measurement of small changes associated with very slow motions in a material (see Inelastic scattering).

NEUTRON DIFFRACTION
Neutrons can be reflected, or scattered, off a material in which the interatomic distances are similar to the neutron wavelength. The scattered waves interfere to produce a characteristic diffraction pattern. In standard neutron diffraction, a single crystal is oriented over a range of angles to collect neutron beams diffracted from different planes of atoms in the crystal.

NEUTRON IMAGING
The use of neutrons to obtain a non-destructive radiographic image of the interior of an object by detecting the differential attenuation of the transmitted neutron beam.

NEUTRON REFLECTOMETRY
A technique in which neutrons are reflected off a surface or interface. It is used to characterise the structure of surfaces and thin layers.

NEUTRON SPIN ECHO
A neutron technique which measures the changes in the spins of neutrons passing through a material, caused by small changes in energy associated with molecular movements over relatively long time-scales.

NEUTRON STRAIN IMAGING
A method of using neutron diffraction to create a 3D image of the 'strain' in the interior of engineering structural components, obtained by measuring small changes in the spacings of planes of the constituent atoms.

NEUTRON TIME-OF-FLIGHT SPECTROSCOPY
A spallation-source-based technique for measuring the energies of neutrons scattered by a sample, by measuring the time taken for the neutrons to reach the detector (higher-energy neutrons travel faster). The energy exchanged between neutrons and the sample materials can be used to infer the motion and dynamics of the atoms in the material (see also Triple-axis spectroscopy).

NEUTRON TOMOGRAPHY
A form of non-destructive neutron imaging in which a series of radiographic image 'slices' through an object are taken and combined to reconstruct a three-dimensional representation (similar to computer-aided X-ray tomography, or CAT).

POLARISED NEUTRONS
A beam of neutrons whose spins are all aligned.

POLARISED NEUTRON DIFFRACTION
A class of neutron experiments using polarised neutrons to investigate the magnetic properties of materials.

POLARISED NEUTRON REFLECTOMETRY
A technique using polarised neutrons (whose spins are aligned) to investigate magnetic properties at surfaces and interfaces in a reflection geometry.

POLYMER
A molecule comprising repeating molecular units (monomers) usually in long chains.

POWDER DIFFRACTION
The coherent, elastic scattering of neutrons from a polycrystalline material to give a characteristic diffraction pattern that can be used to analyse the atomic structure of a material (see also Wide-angle scattering and Neutron diffraction).

PROTEIN
A long chain of amino acids. Each protein has a specific amino-acid sequence which causes it to fold up into a unique three-dimensional structure with a unique biological function.

QUANTUM FLUCTUATION
The mathematics underpinning quantum theory predicts that there is always a small uncertainty in connected properties such as position and momentum, or energy and time. This results in inherent fluctuations in quantum states, for example, spin states that are similar in energy.

QUANTUM STATE
Systems obeying the laws of quantum mechanics, such as particles or nuclei, exist in defined energy states.

QUANTUM TUNNELLING
Quantum particles can traverse, or 'tunnel' through an energy barrier because the Uncertainty Principle of quantum mechanics predicts that there is always a small probability of them being located on the other side.

RESIDUAL STRESSES
A manufactured material retains interior stresses (forces) at the atomic level – which are present even in the absence of external loads.

SHEAR STRAIN
The effect of an applied force whereby parallel internal surfaces of a material are made to slide over one another, thus inducing a shear stress (force).

SMALL ANGLE NEUTRON SCATTERING (SANS)
The measurement of neutron scattering at small angles, used to investigate objects and structures such as polymers or biological molecular arrangements of the order of tens or hundreds of nanometres.

SPIN
The term describing the internal angular momentum of a quantum particle such as the electron or neutron, or of an assembly of particles such as a nucleus.

SPIN GLASSES AND SPIN ICES
A magnetic state of a material in which the spins (electron magnetic moments) are disordered and are continually changing direction over time, as a result of geometrically conflicting interactions trying to align them (frustration). A spin ice retains the residual geometric frustration at very low temperatures.

SUPERALLOY
An alloy with a high mechanical strength at high temperatures, and resistance to corrosion.

SUPERCONDUCTOR
A material that has no electrical resistance below a certain temperature and which can therefore conduct electricity loss-free.

TRIPLE AXIS SPECTROSCOPY
A technique using equipment that allows the energy of scattered neutrons to be measured in all directions to provide information about the atomic motion.

VISCOELASTIC MATERIAL
A material that exhibits both viscous and elastic properties when a deforming force acts on it.

WIDE ANGLE NEUTRON SCATTERING
The measurement of neutron scattering at wide angles, using diffraction in order to investigate the structure and properties of the material at the atomic level.

WELDING
A wide variety of processes in which materials, such as metals or plastics, are joined by bringing their edges together; a molten seam is created that solidifies when cooled.

NEUTRON–SCATTERING TECHNIQUES

Scientists working with neutrons have developed a sophisticated toolbox to extract information about the structure and behaviour of materials – from metals to living cells – across a wide range of length and time-scales. In a typical experiment, a beam of neutrons, prepared with a particular direction, energy (velocity) and spin orientation, impinges on a sample. The scattered neutrons are then collected in a detector which measures their new directions, energies and spin states. The types of methods and instruments chosen depend on the problem being solved, or sample studied. Higher-energy neutron beams ('hot' neutrons) are used to study structures and fast movements at the atomic scale, while lower-energy beams ('cold' neutrons) are suitable for studying larger structures and slower dynamics, such as the shape of protein molecules and how they move.

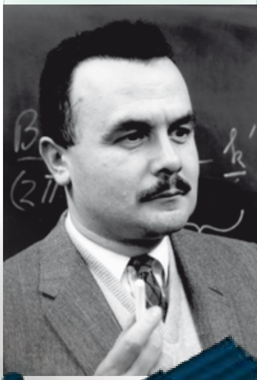
NEUTRON DIFFRACTION: the pattern of neutrons (numbers and angles) scattered from a sample provides information on the relative positions of the constituent atoms or molecules.

SMALL ANGLE NEUTRON SCATTERING (SANS): measuring scattering at very small angles, using specially designed, very long instruments, gives information about large-scale structures, such as molecular assemblies in biological cells and composite materials.

NEUTRON REFLECTOMETRY: reflecting a neutron beam from a surface, or interface, produces intensity patterns corresponding to structure close to that surface.

POLARISED NEUTRON SCATTERING: the spins of neutrons can be aligned to produce a polarised neutron beam. Detecting how the alignments change as the neutrons are scattered gives information on magnetic structure and dynamics.

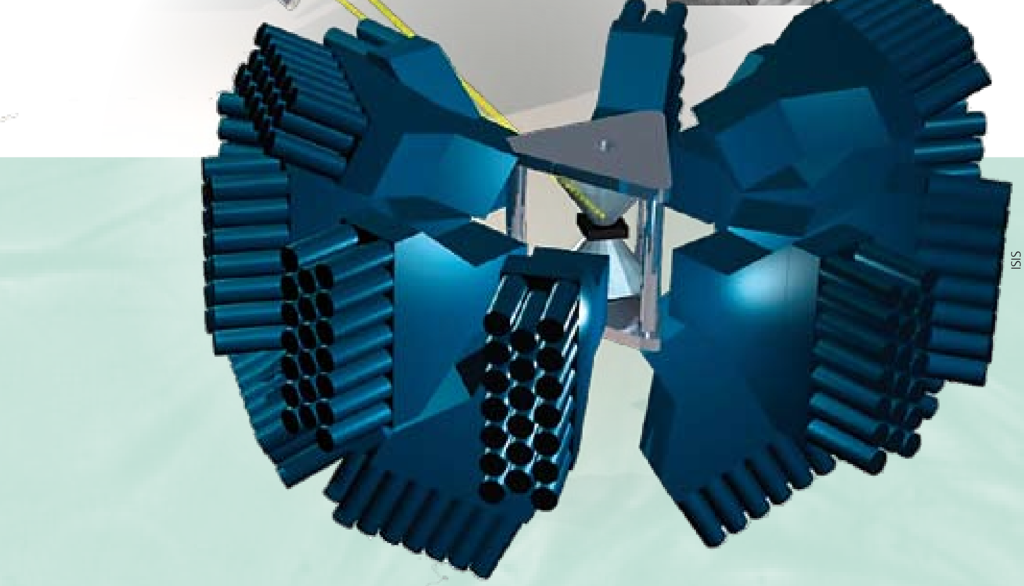
Cifford Shull (above) and Bertram Brockhouse (below) who won the Nobel Prize for Physics in 1994 for the development of neutron-scattering techniques http://nobelprize.org/nobel_prizes/physics/laureates/1994



INELASTIC NEUTRON SCATTERING: measuring the changes in neutron energies following scattering provides information on dynamic changes at the atomic and molecular level relevant to atomic quantum states, vibrations and bond strengths, and molecular motion.

NEUTRON SPIN ECHO: much slower dynamics associated with large molecular structures such as polymer molecules can be accessed via polarised neutrons rotating at a given frequency, which then behave like a 'clock'. Measuring how the clock-time changes as the neutron beam is scattered gives information about energy changes at this time-scale.

NEUTRON RADIOGRAPHY: like X-rays, neutrons transmitted through an object can give either a 2D or a 3D image (as in a hospital CT scan) of the internal structure.



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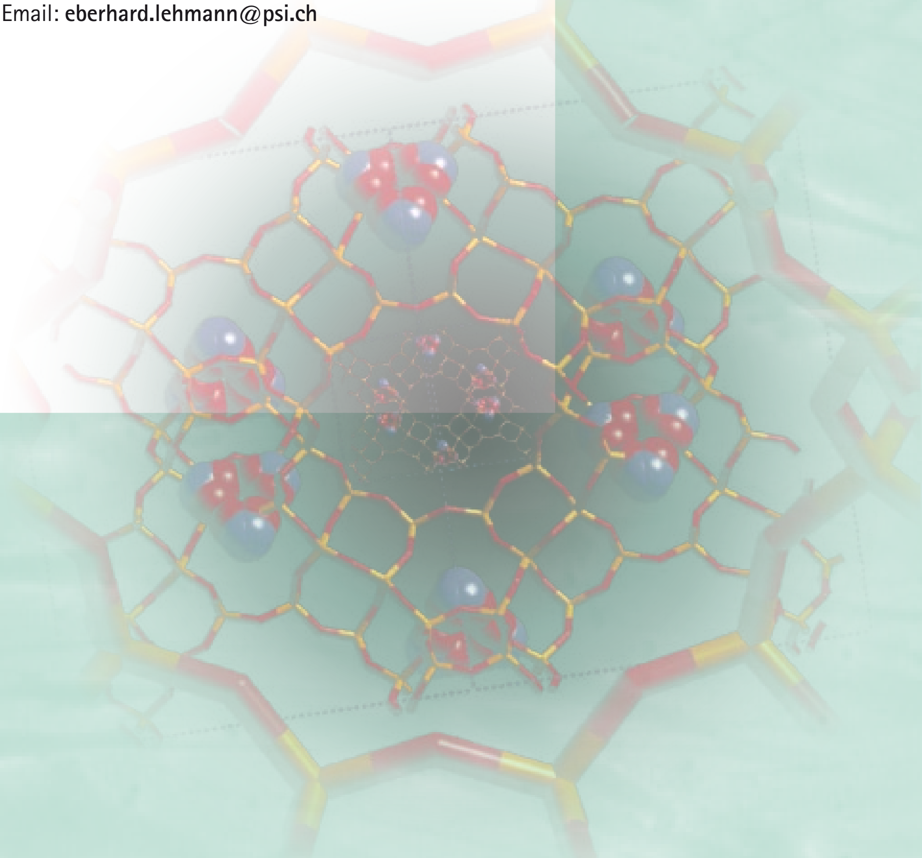

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